Strain and the Thermodynamics of Buried AlGaAs Layer Oxidation

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Outline

- Buried oxide layers in AlGaAs/GaAs heterostructures
- Electron backscatter diffraction for strain mapping
- Thermodynamic calculations of phases
- Future studies

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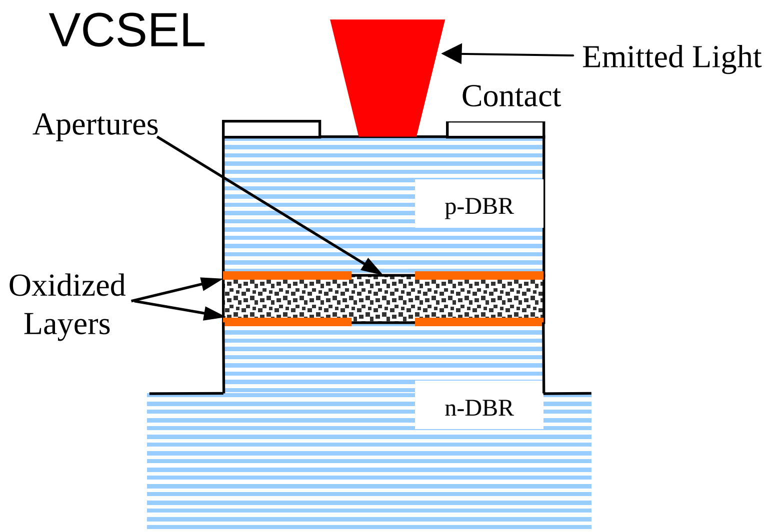
$Al_xGa_{1-x}As$ Native Oxides



Device Applications

- Vertical cavity surface emitting lasers (VCSELs)
- Light emitting diodes (LEDs)
- Edge emitting lasers
- Distributed bragg reflectors (DBRs)
- Field effect transistors (FETs and MOSFETs)

Mechanical Reliability Issue

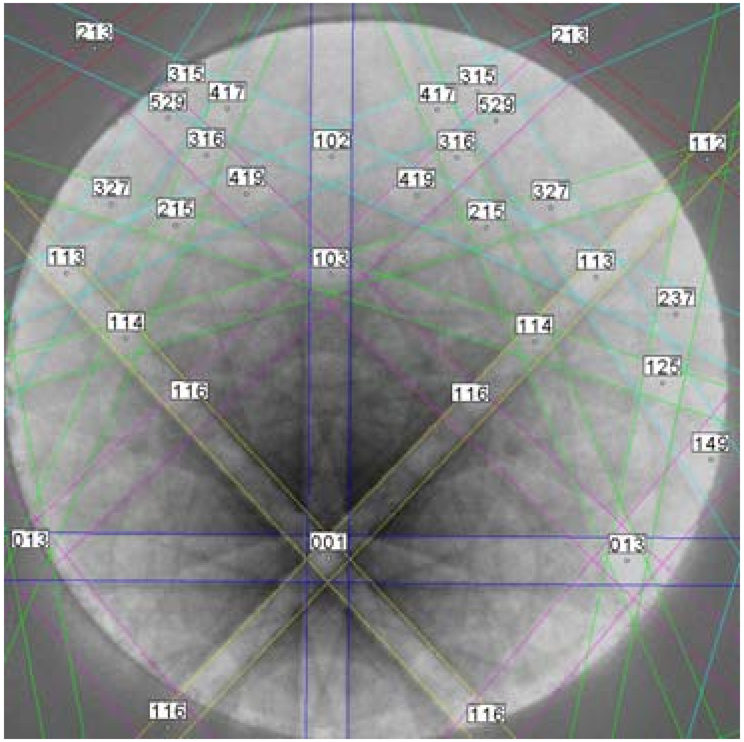
- Large elastic strains associated with oxide formation.
- Shrinkage of constrained $Al_{0.98}Ga_{0.02}As$ layers ~7%
  measured by TEM, R.D. Twesten et al. APL 69 [1] 19-21 (1996).
- Leads to device failure.
- Strain mapping requires high spatial resolution technique.

Electron Backscatter Diffraction

- Performed in FESEM
- Spatial resolution for GaAs ~30 nm (at 15 kV).

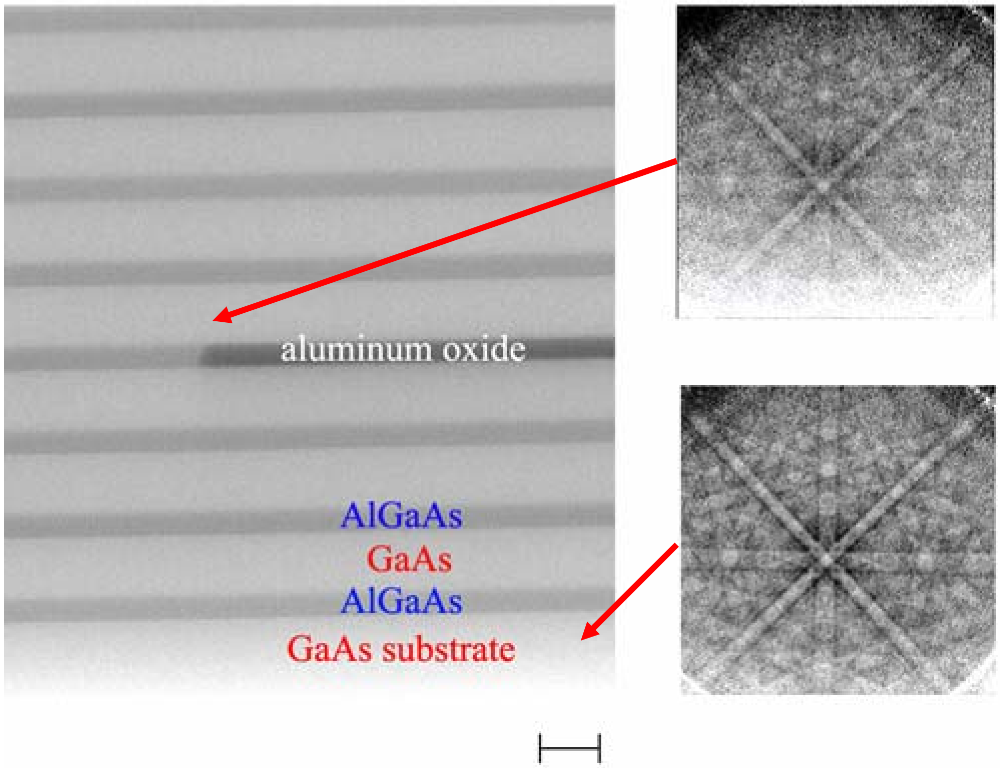
  depends on information volume of backscattered electrons (Z and keV)
- Kikuchi bands.
- Width of bands proportional to Bragg angles (lattice parameters).

  $W = 2 \cdot \theta_{hkl} \qquad \theta_{hkl} = \arcsin(n\lambda/2d_{hkl})$
- Relative strain of 0.2 % detectable.
- Strain gradients cause continuously changing lattice parameters – broaden band edges.



Indexed GaAs EBSD pattern

EBSD Measurement of Strain Gradients



200 nm

Pattern close to oxide interface

Pattern far from oxide interface

Diffuseness indicates larger strain gradient near oxide interface.

FESEM image of multilayer structure.

EBSD patterns from GaAs.

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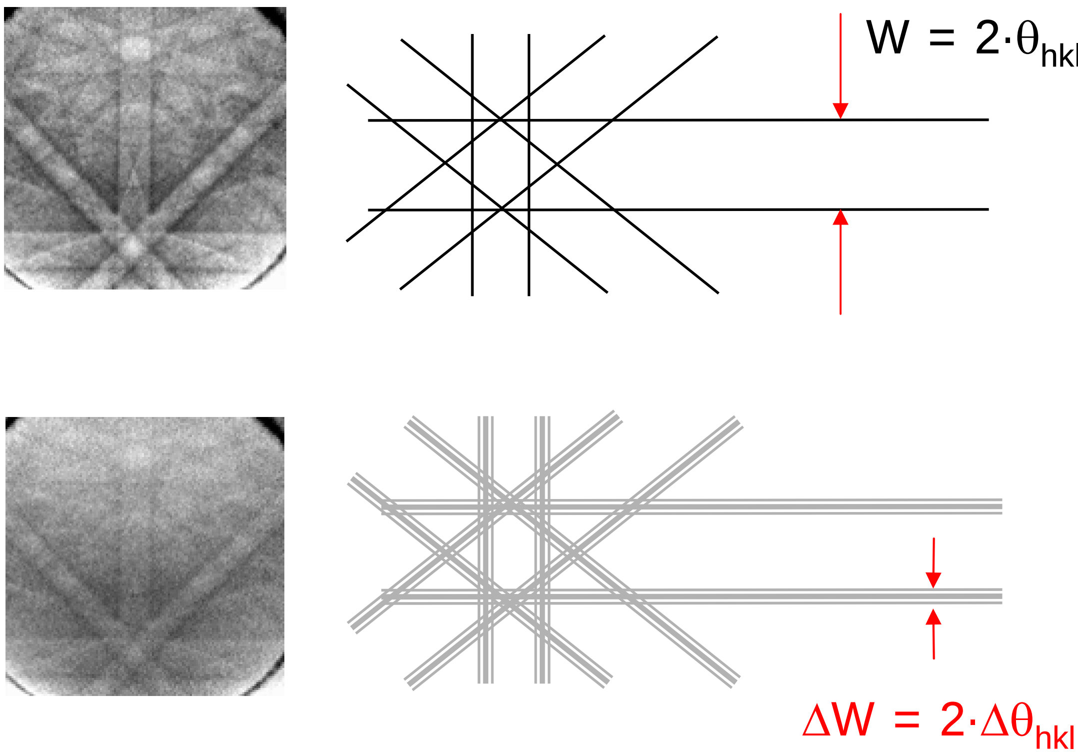
Elastic Strain Gradients and Width of Band Edges



- Strain gradient causes variation in d(hkl) leading to $\Delta\theta_{hkl}$.
- Line edges become diffuse.
- Maximum (and average) band intensity decreases.

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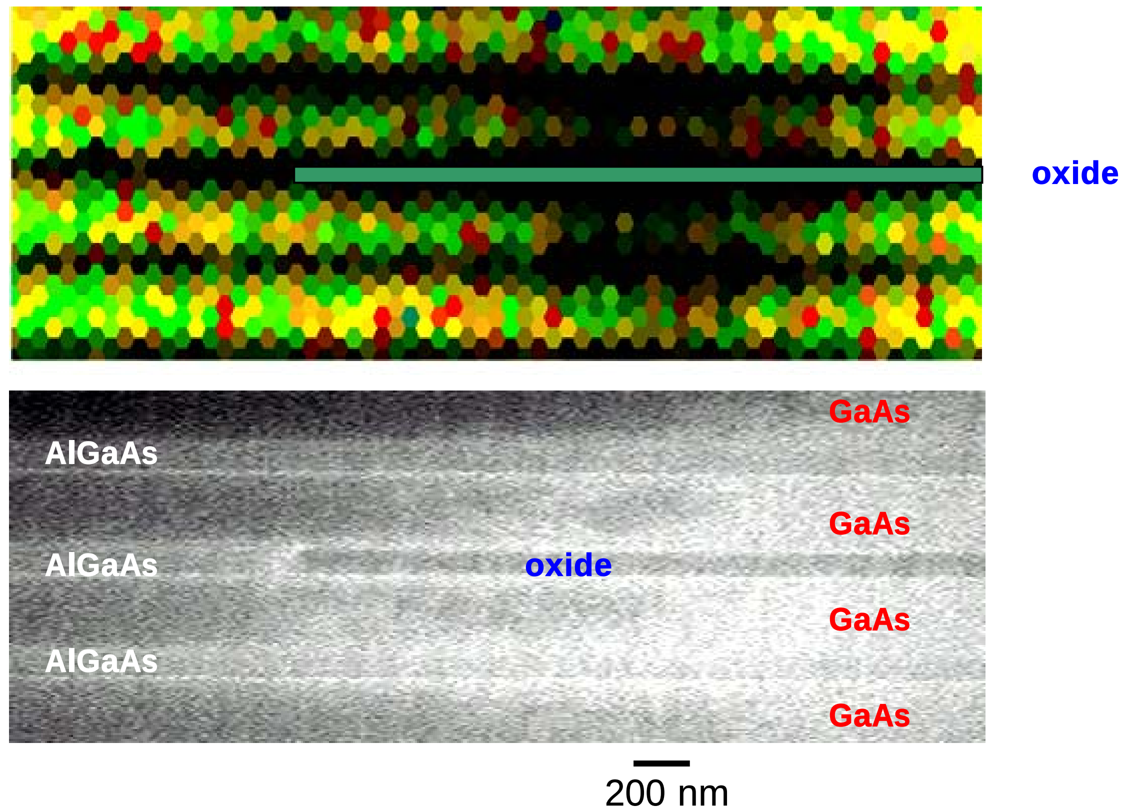
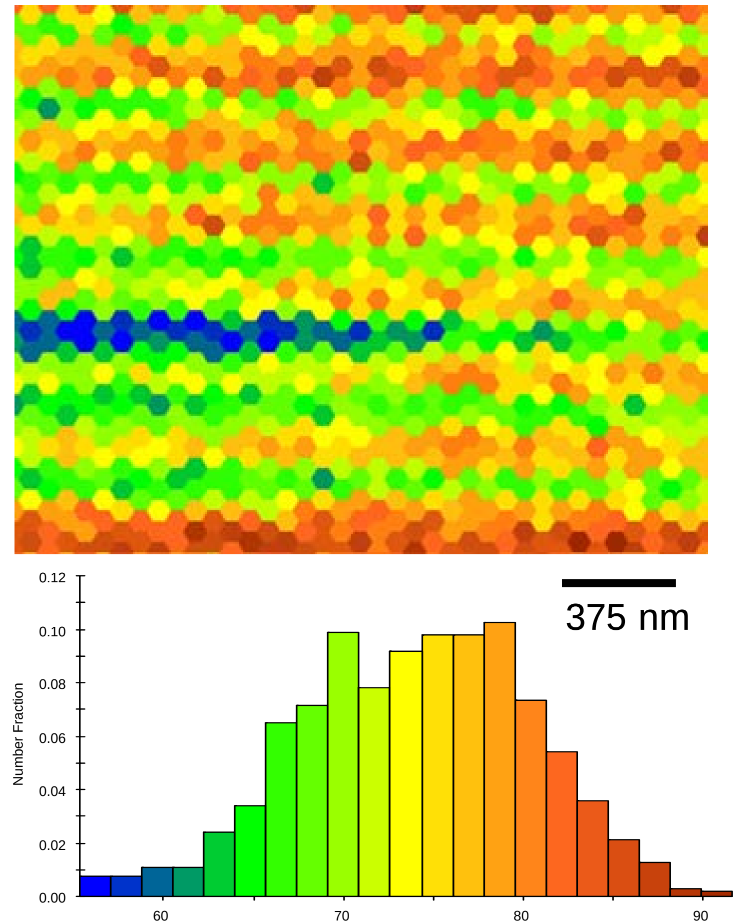
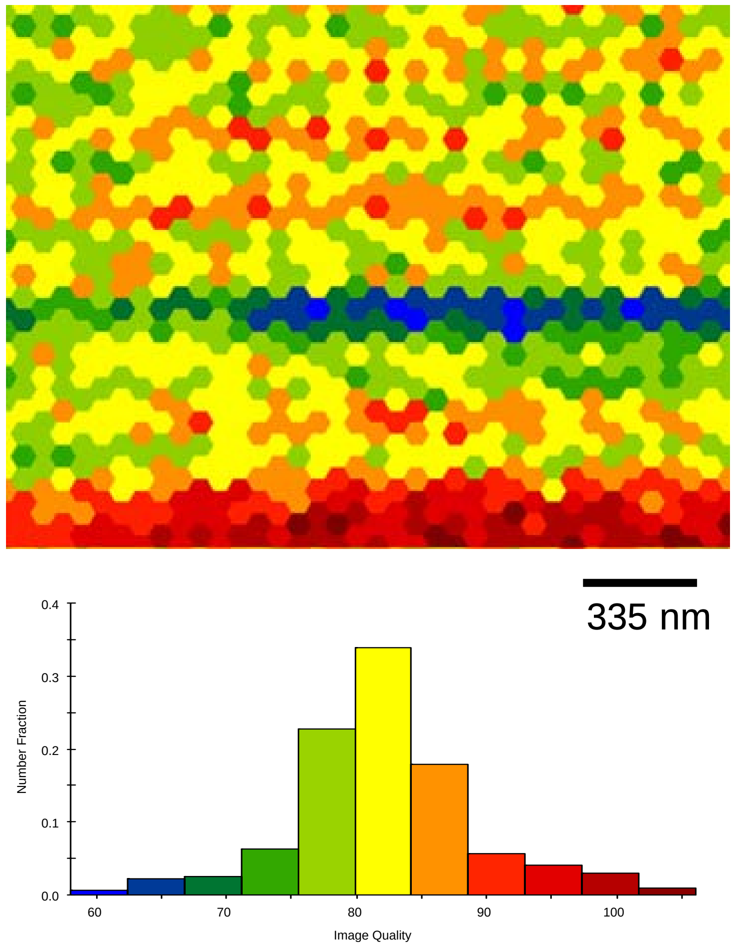
EBSD Mapping of Strain Gradients

- Map of image quality.
- Darker pixels indicate greater pattern diffuseness (larger strain gradients).
- Largest strain gradient behind oxide interface.



Strain Gradient Maps





Thermodynamically Stable Phases

Oxidation in Air (from 0 to 500 ˚C)

$$2\ GaAs(s) + 4\ O_2(g) = Ga_2O_3(s) + As_2O_5(s)$$

$$AlAs(s) + 2\ O_2(g) = AlAsO_4(s)$$

Oxidation in Water Vapor (from 0 to 500 ˚C)

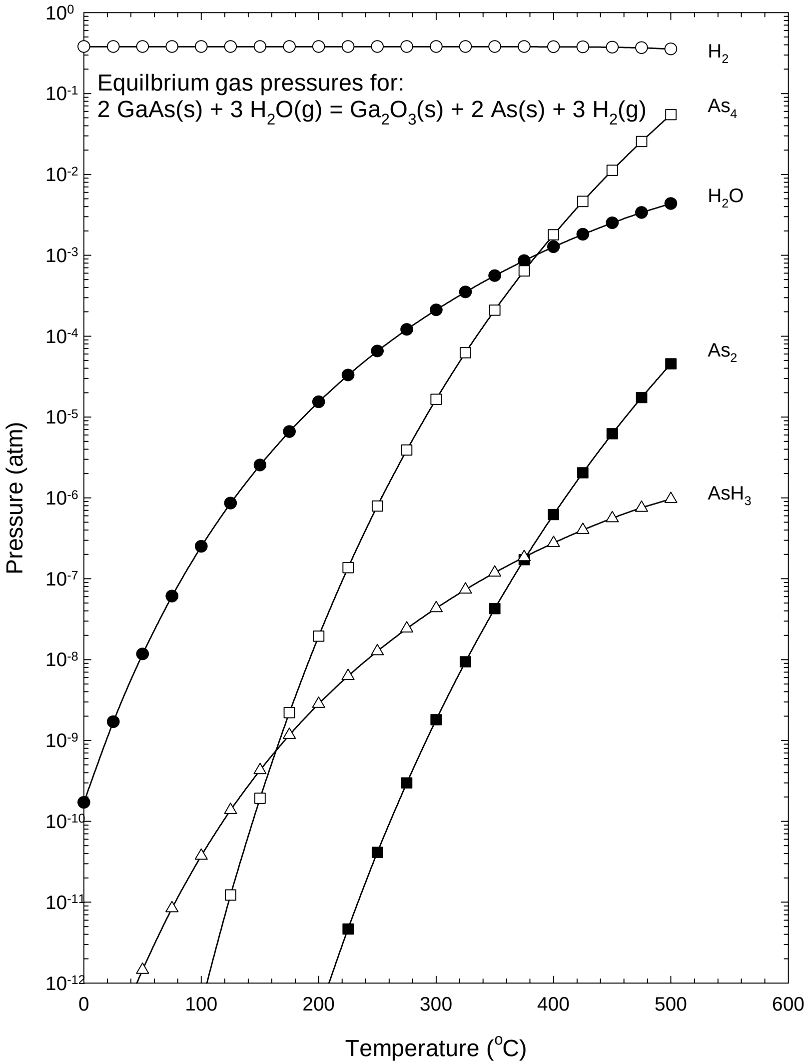
$$2\ GaAs(s) + 3\ H_2O(g) = Ga_2O_3(s) + 2\ As(s) + 3\ H_2(g)$$

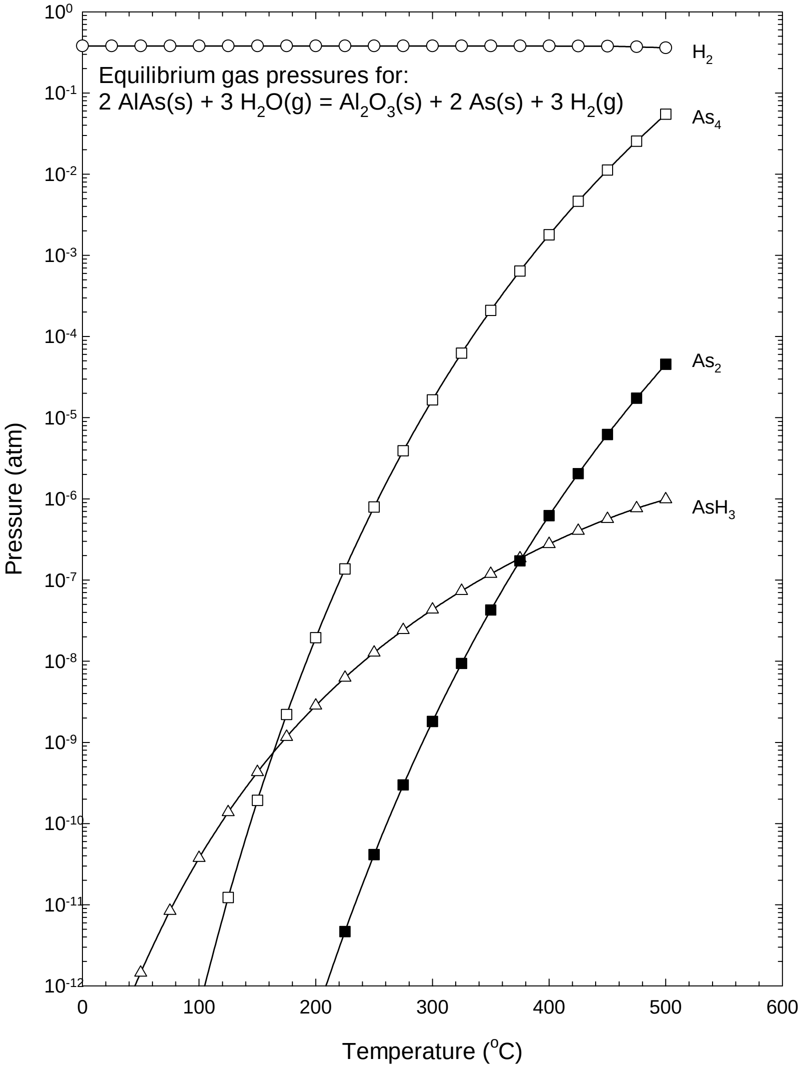
$$2\ AlAs(s) + 3\ H_2O\ (g) = Al_2O_3(s) + 2\ As(s) + 3\ H_2(g)$$

Stable species at 450 °C and 0.38 atm H_2O:

Al_2O_3 : As_4 : Ga_2O_3 (not hydroxides)

Equilibrium Partial Pressures



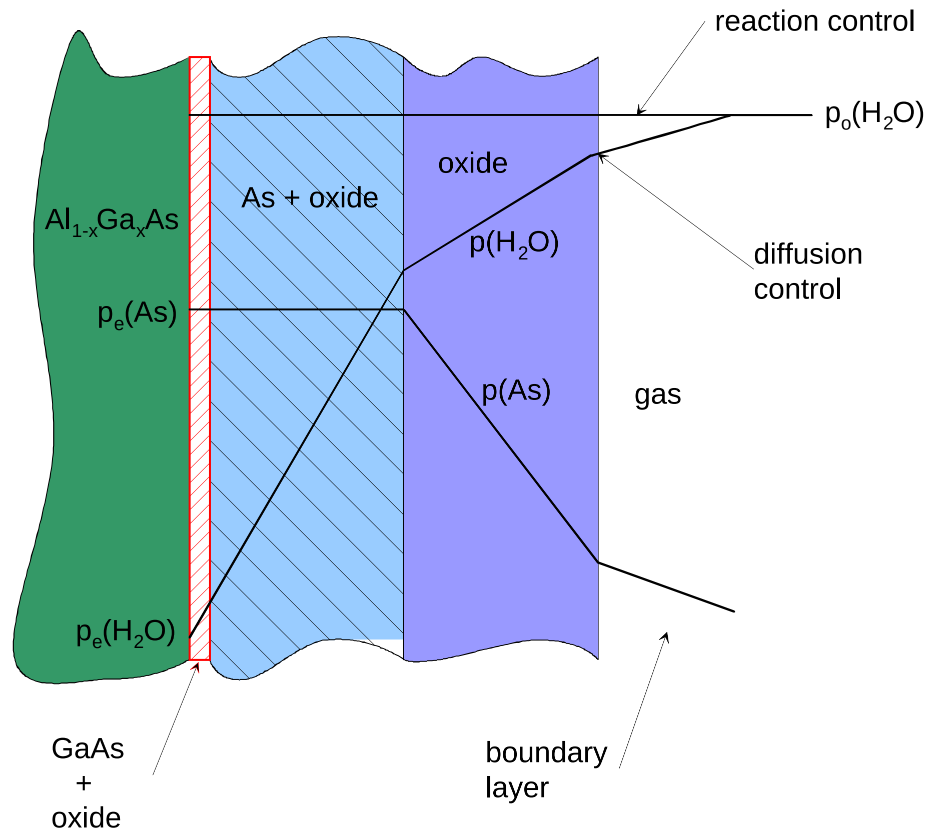


Phases Predicted by Thermodynamics

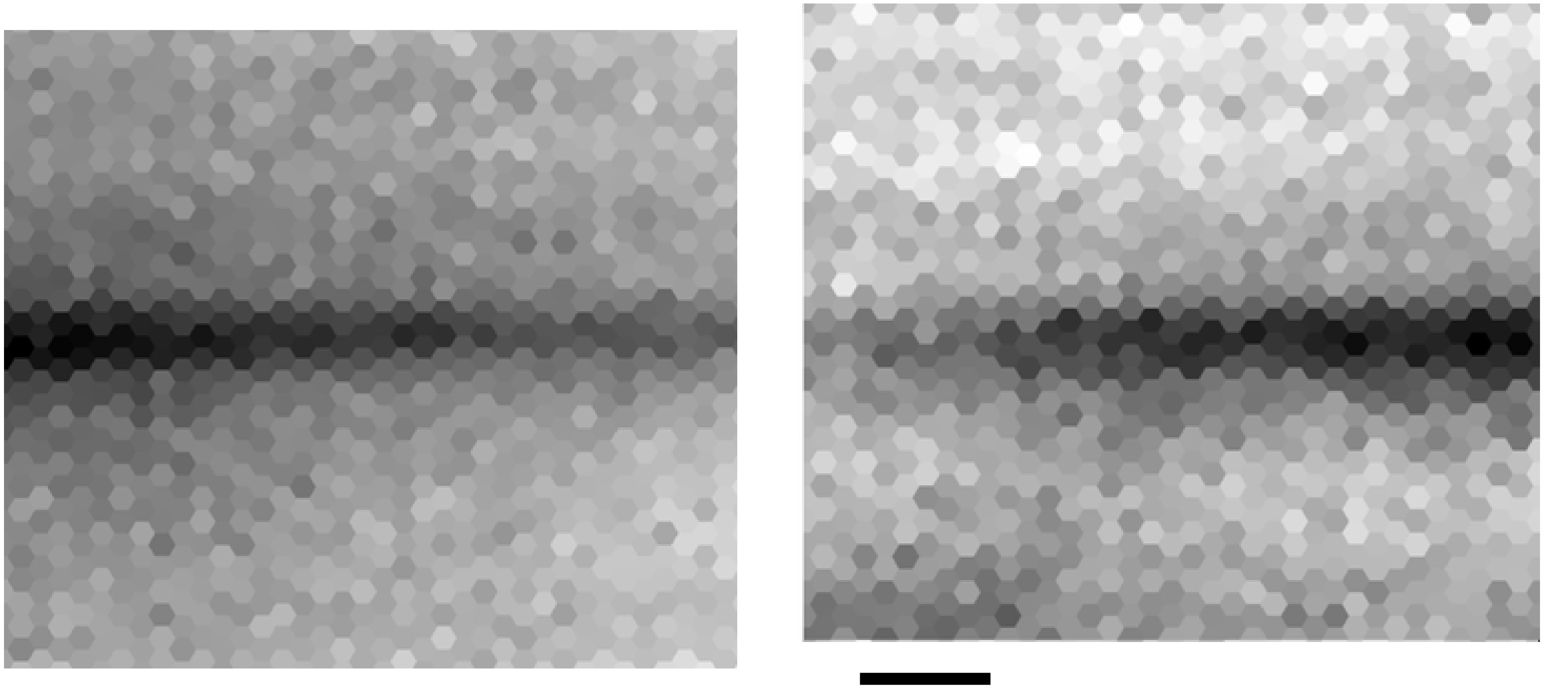
- Equilibrium water vapor pressure over AlAs $>10^9$ times lower than that over GaAs.
- At oxide interface AlAs oxidized, GaAs not.
- Equilibrium water vapor pressure for oxidation of GaAs at 450 ºC ~4.5 x 10-3 atm.

Our samples oxidized at 450 ºC
2.5 l/min N_2 bubbling through water at 75 ºC

(equivalent to 0.38 atm H_2O).



Strain Gradient Map of VCSEL Structure



Oxide and strain field tapered in VCSEL structure material.*

*Material provided by IQE.

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Summary

- Mapping of strain gradients with EBSD.
- Strain gradient largest behind oxide – non-oxide interface for ~80 nm thick layers with no composition gradient.
- Thermodynamics predict As containing region near oxide interface (no contraction), As depleted region ~1 µm behind oxide interface.
- Strain field consistent with thermodynamic model for oxidation.